# Chemical Reaction Engineering Modeling and Simulation in COMSOL Multiphysics®

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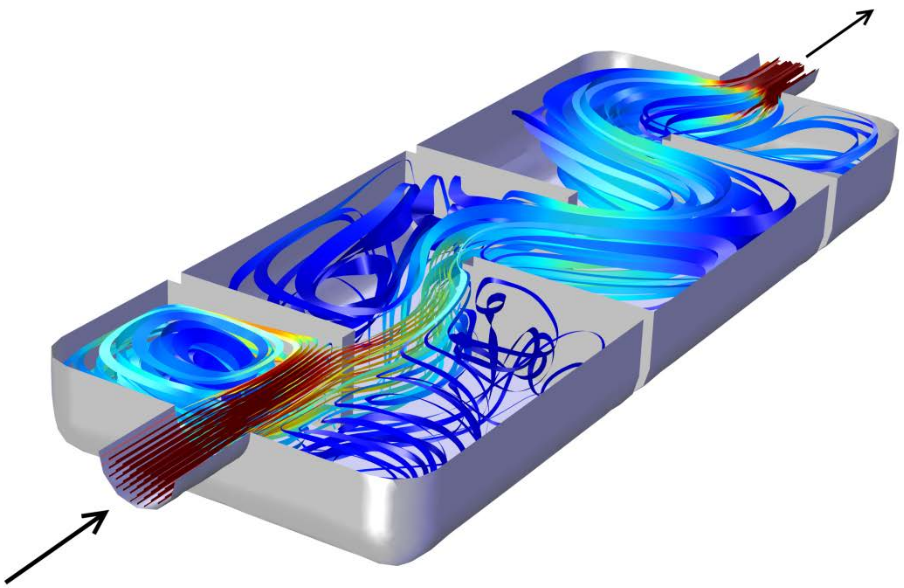

Turbulent reacting flow

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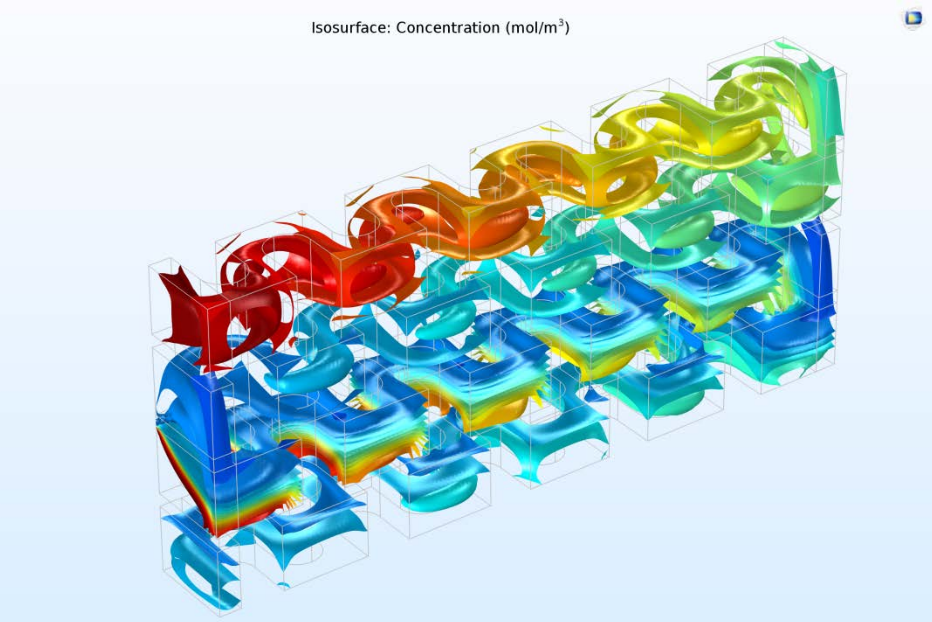
# Why Simulate?

- Understanding
  - Enable intuition for further innovation




Flow and chemical composition in a plate reactor

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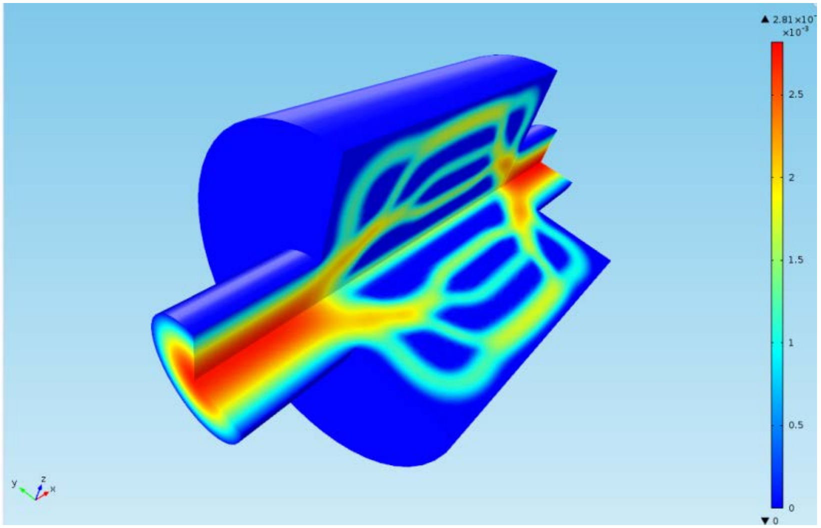
# Why Simulate?

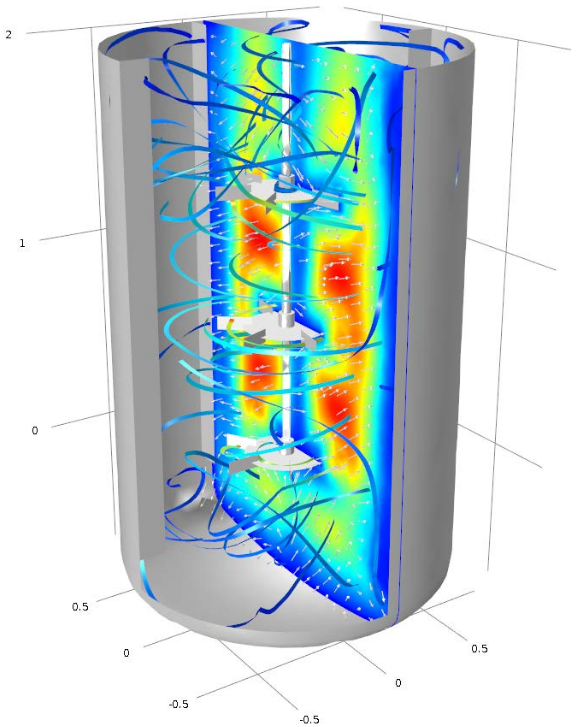
- Understanding
  - Enable intuition for further innovation
- Testing of new ideas




Optimization of a catalytic reactor

# Why Simulate?

- Understanding
  - Enable intuition for further innovation
- Testing new ideas
- Control and optimization
  - Adapt the process to different operating conditions
  - Reduce the need for prototypes and pilot plants




Batch reactor equipped with three Rushton turbines

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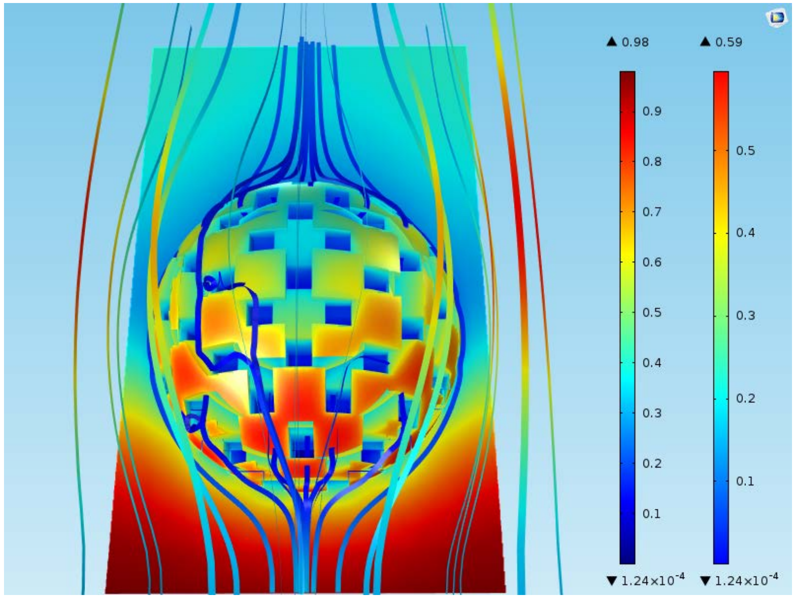
# Why Simulate?

- Understanding
  - Enable intuition for further innovation
- Testing new ideas
- Control and optimization
  - Adapt the process to different operating conditions
  - Reduce the need for prototypes and pilot plants
- Predict the unmeasurable
  - Simulate impossible or dangerous scenarios




Flow and reactions in an idealized porous catalytic particle

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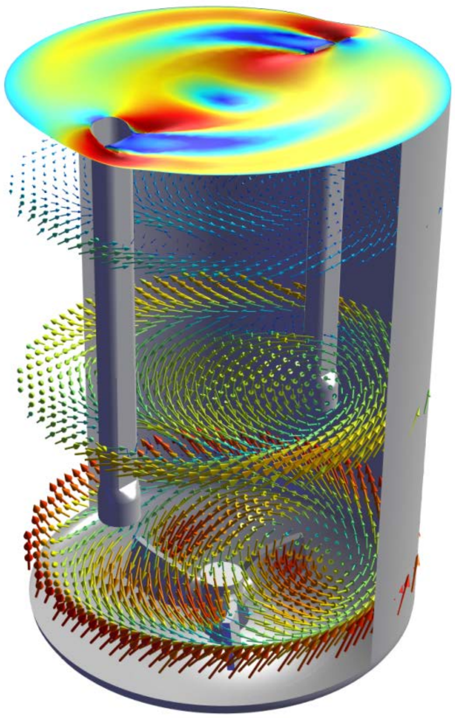
# Why Simulate?

- Understanding
  - Enable intuition for further innovation
- Testing new ideas
- Control and optimization
  - Adapt the process to different operating conditions
  - Reduce the need for prototypes and pilot plants
- Predict the unmeasurable
  - Simulate impossible or dangerous scenarios
- Validation



Reacting flow in a tank equipped with a bottom mixer

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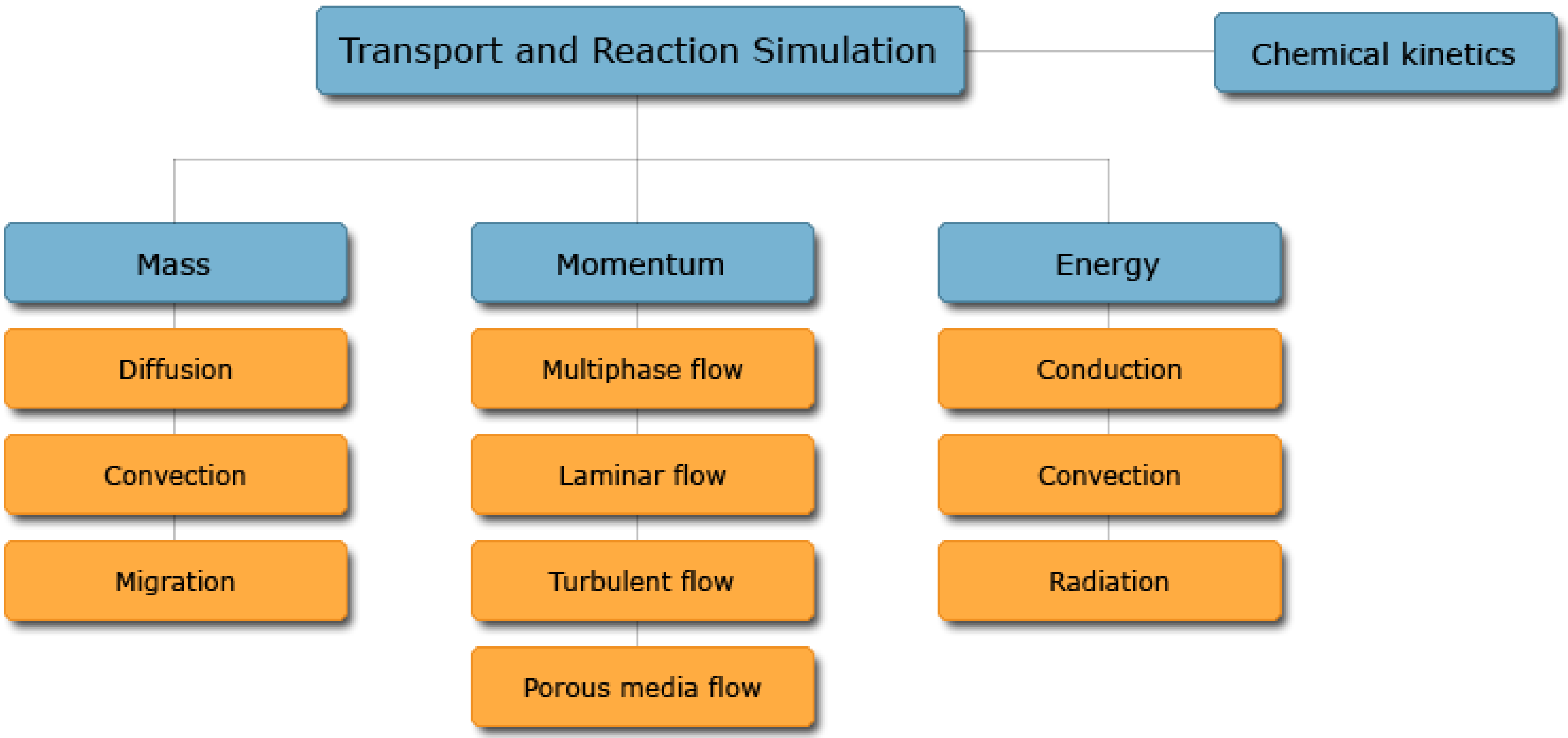
# Mass, Energy, and Momentum

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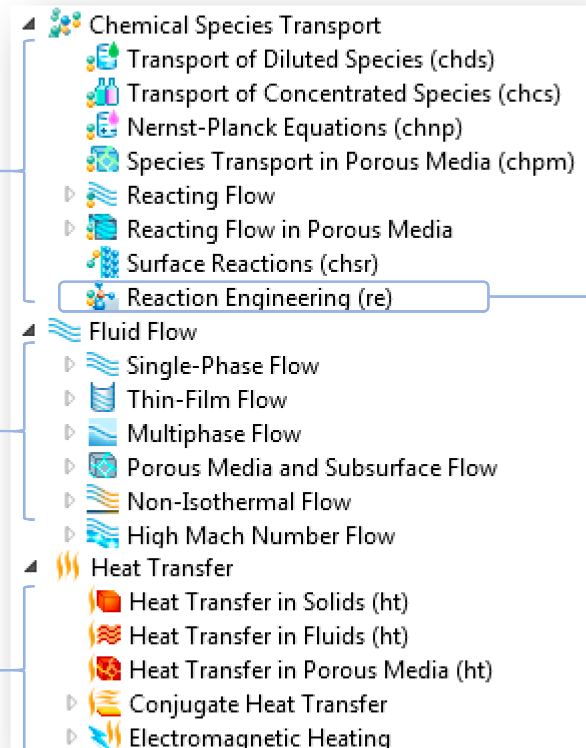
# The Chemical Reaction Engineering Interfaces

Mass Transport and reactions

Momentum Transport (Mass and Energy too)

Energy Transport




Just type in the reaction

Chemical Reaction Engineering Module and CFD Module

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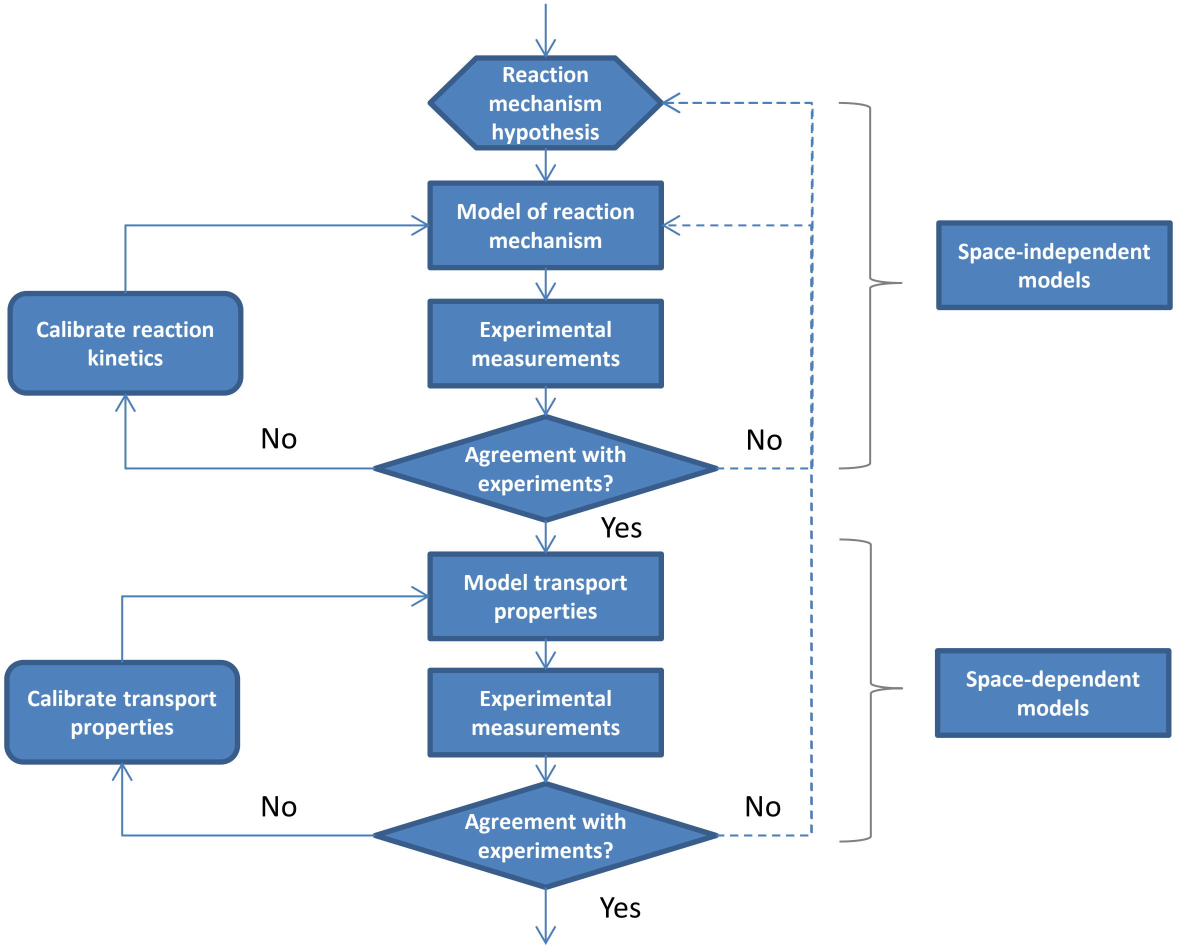
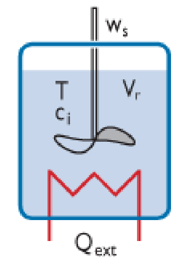
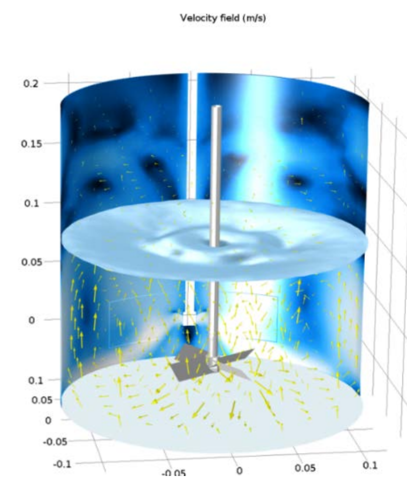
# Modeling Strategy




Space-independent




Perfectly mixed systems




Space-dependent process

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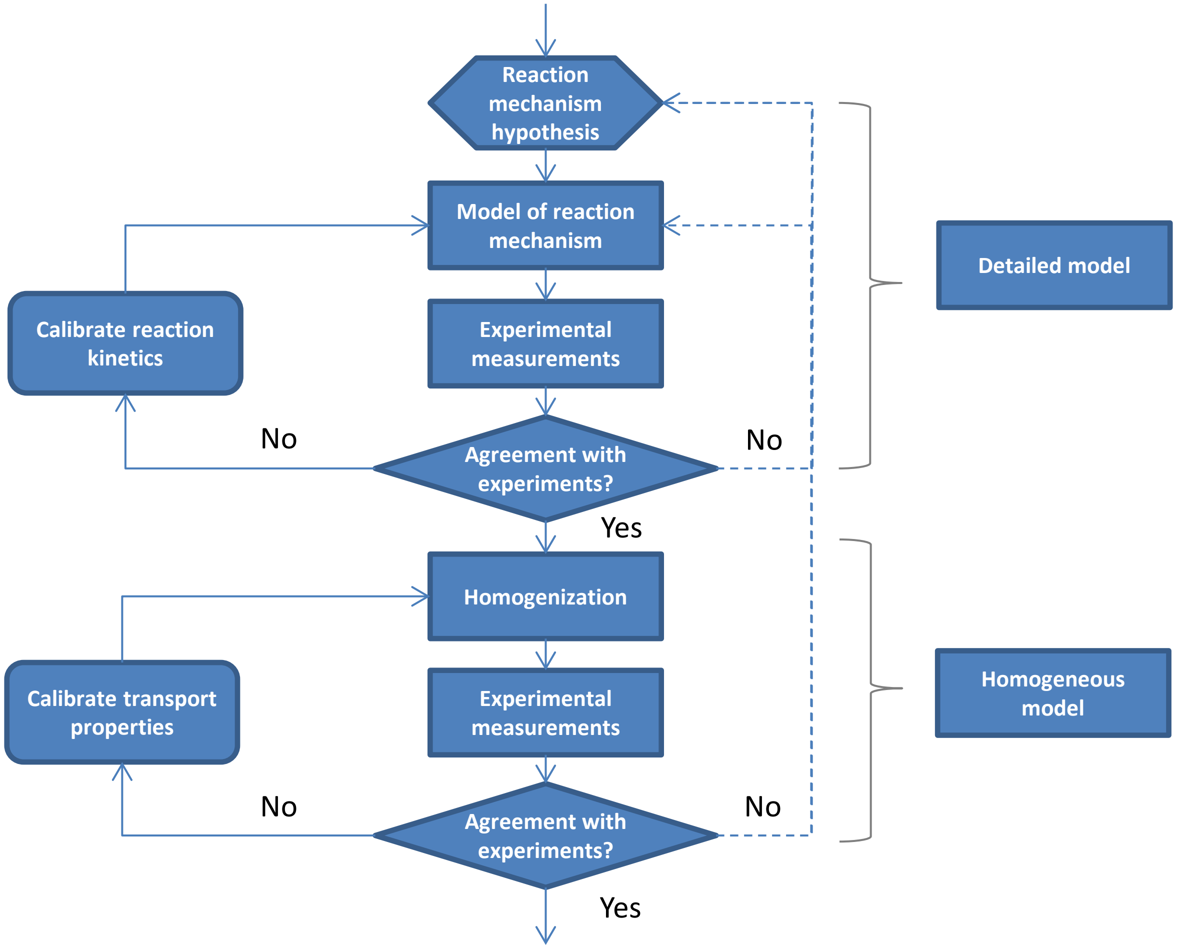
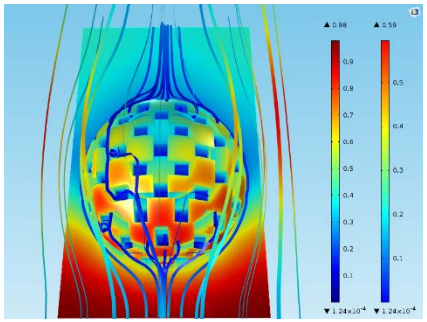
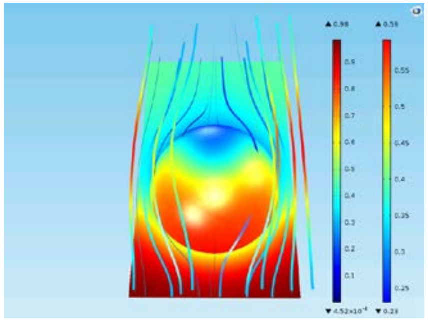
# Modeling Strategy, Heterogeneous Catalysis




Detailed model



Heterogeneous reactions



Homogeneous model

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# Example of the Modeling Strategy with the Chemical Reaction Engineering Module

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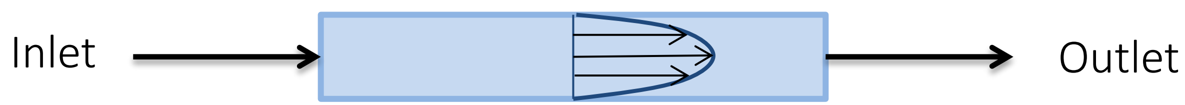
# Reaction Model

- Reaction:

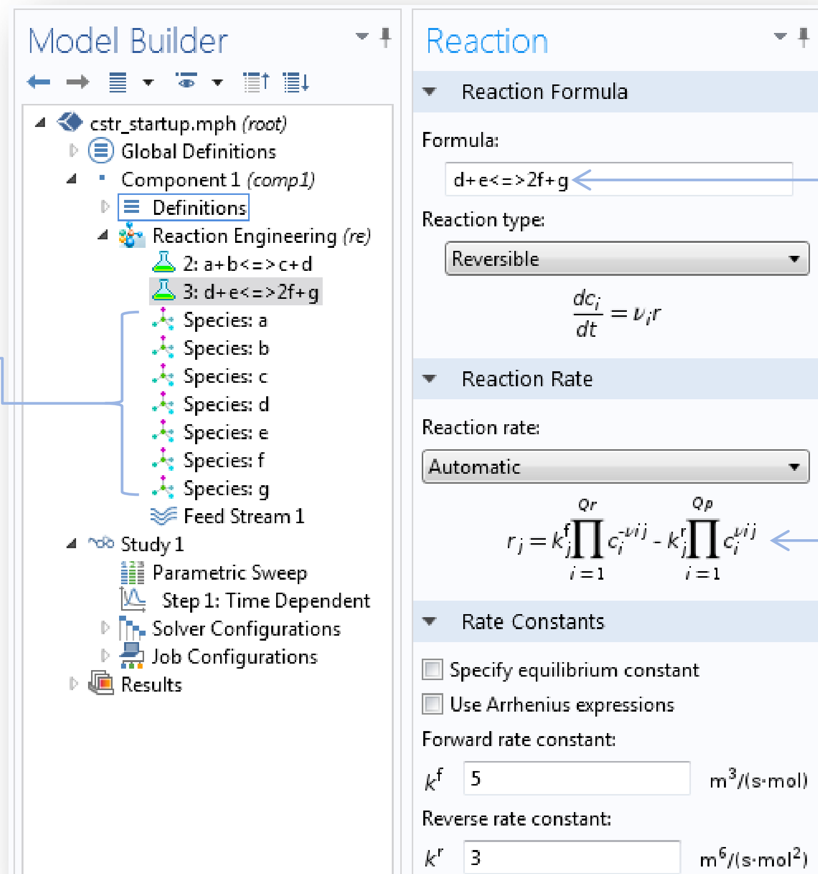
  $a + b \Leftrightarrow c + d$

  $d + e \Leftrightarrow f + g$

- Reactor model:
  - Parallel plate reactor with fully developed laminar flow



# Define Chemical Reaction Formulas in Perfectly Mixed Environment




1. Just type in the chemical reactions

2. The material balances for the species are automatically generated as you type in the chemical equations

3. The kinetics are automatically formulated according to the mass-action law. If needed, you can replace the rate law with your own expressions

4. Automatic units of rate constants, depending on kinetics expressions

Models for batch, semi-batch, continuous stirred tank reactors, and plug-flow reactors are predefined

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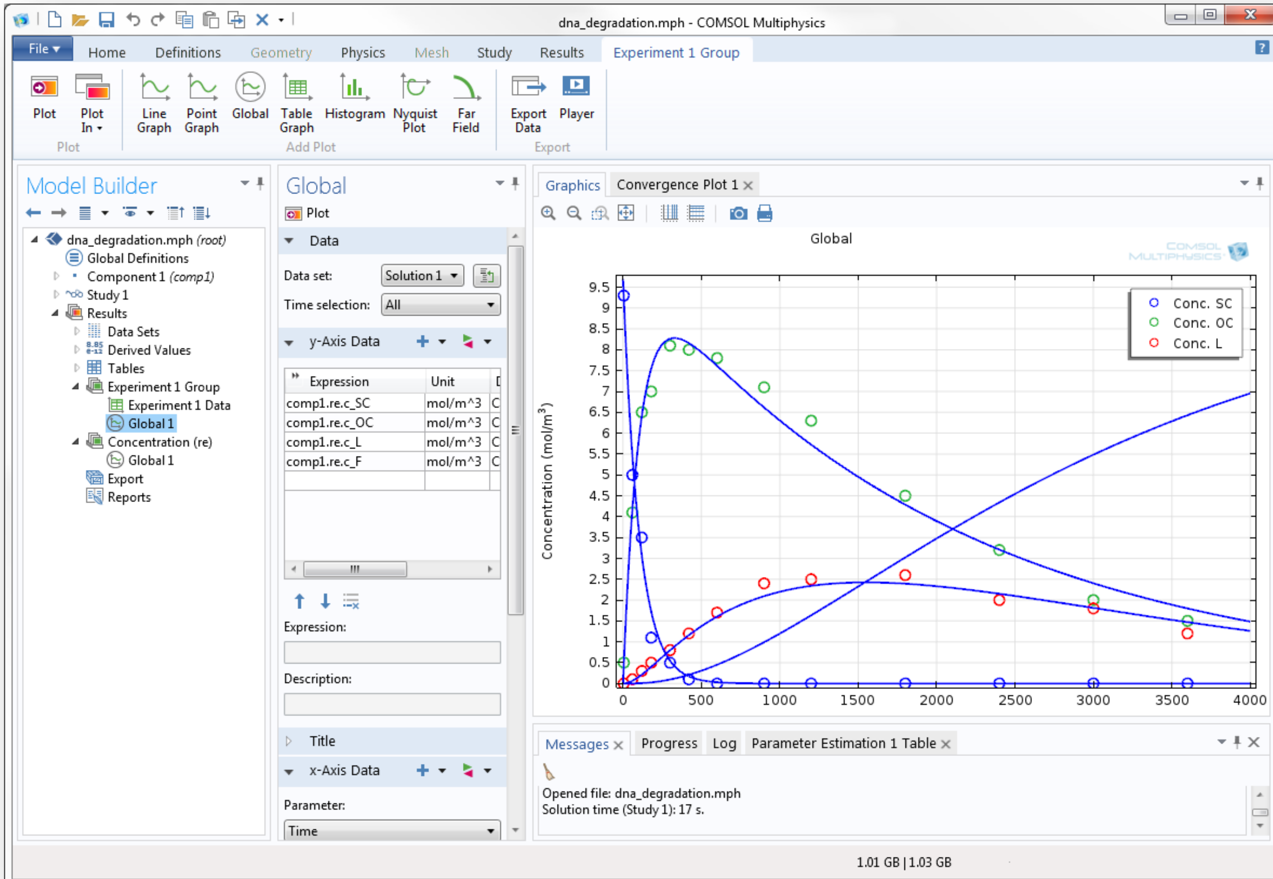
# Simulation and Parameter Estimation
# Ideal Batch Reactor

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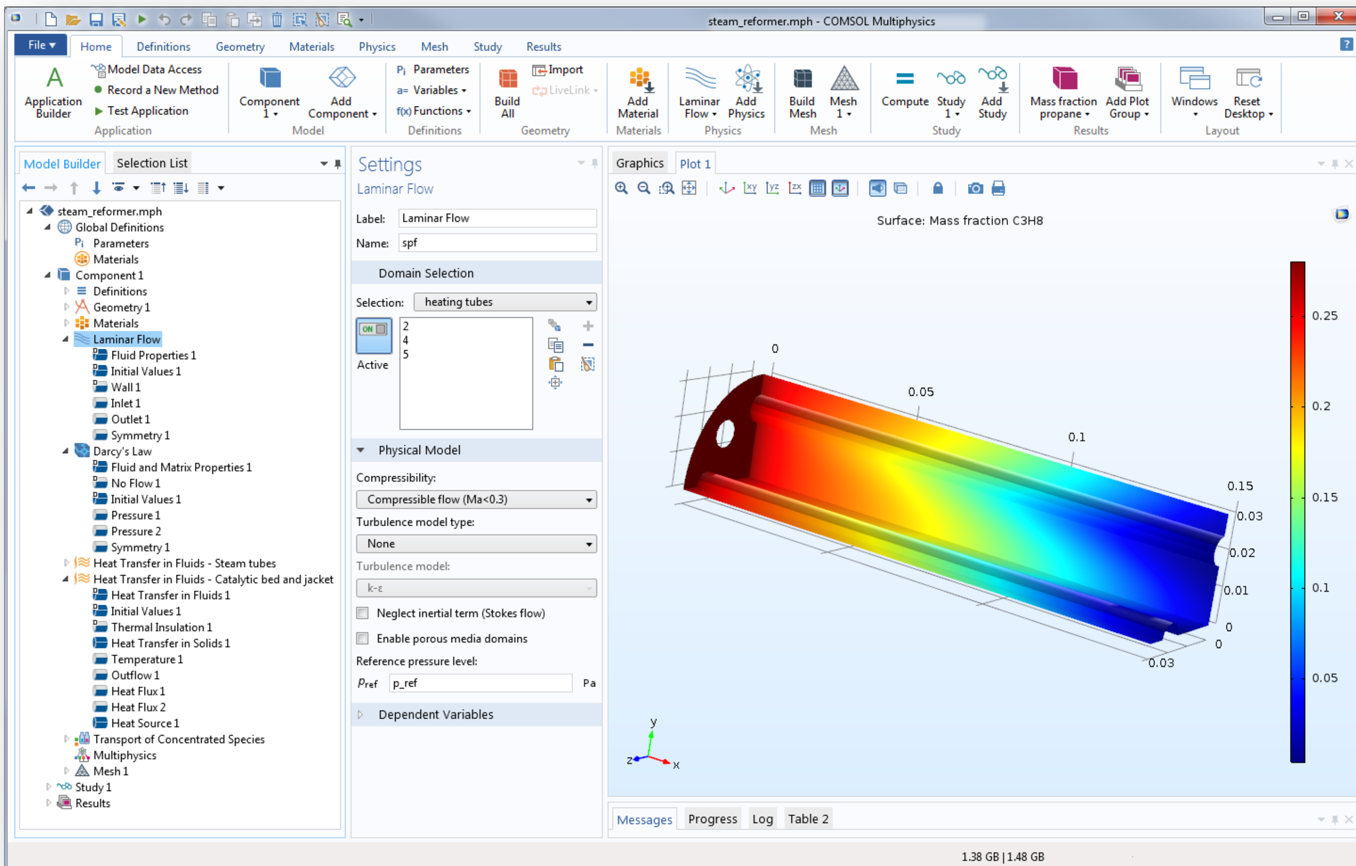
# Extend to Space-Dependent Models of Non-Ideal Reactors



# Example of the Modeling Strategy for Heterogeneous Catalysis

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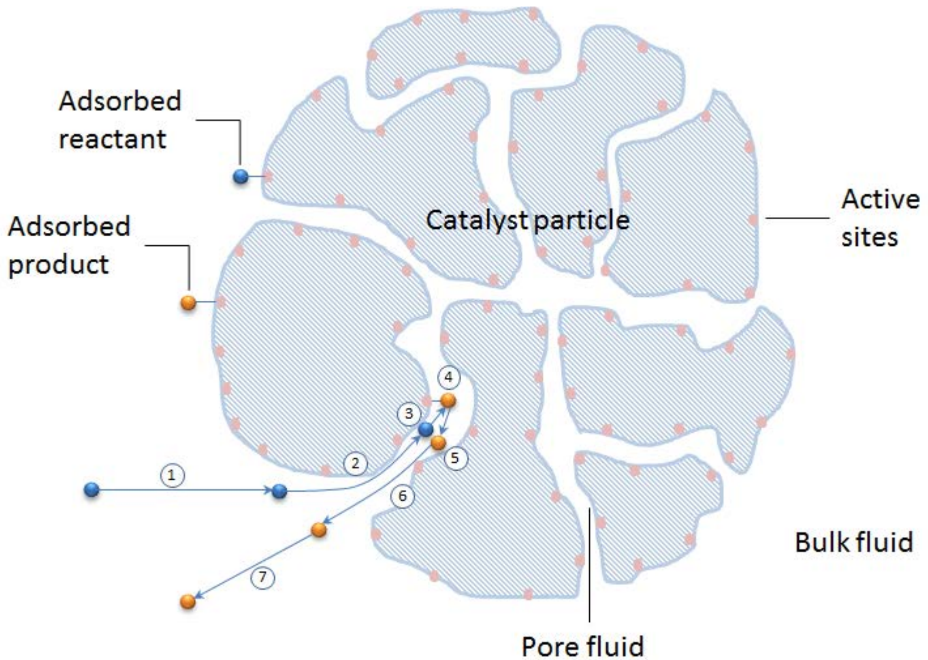
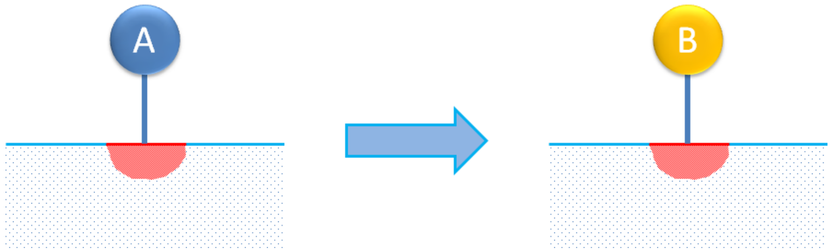
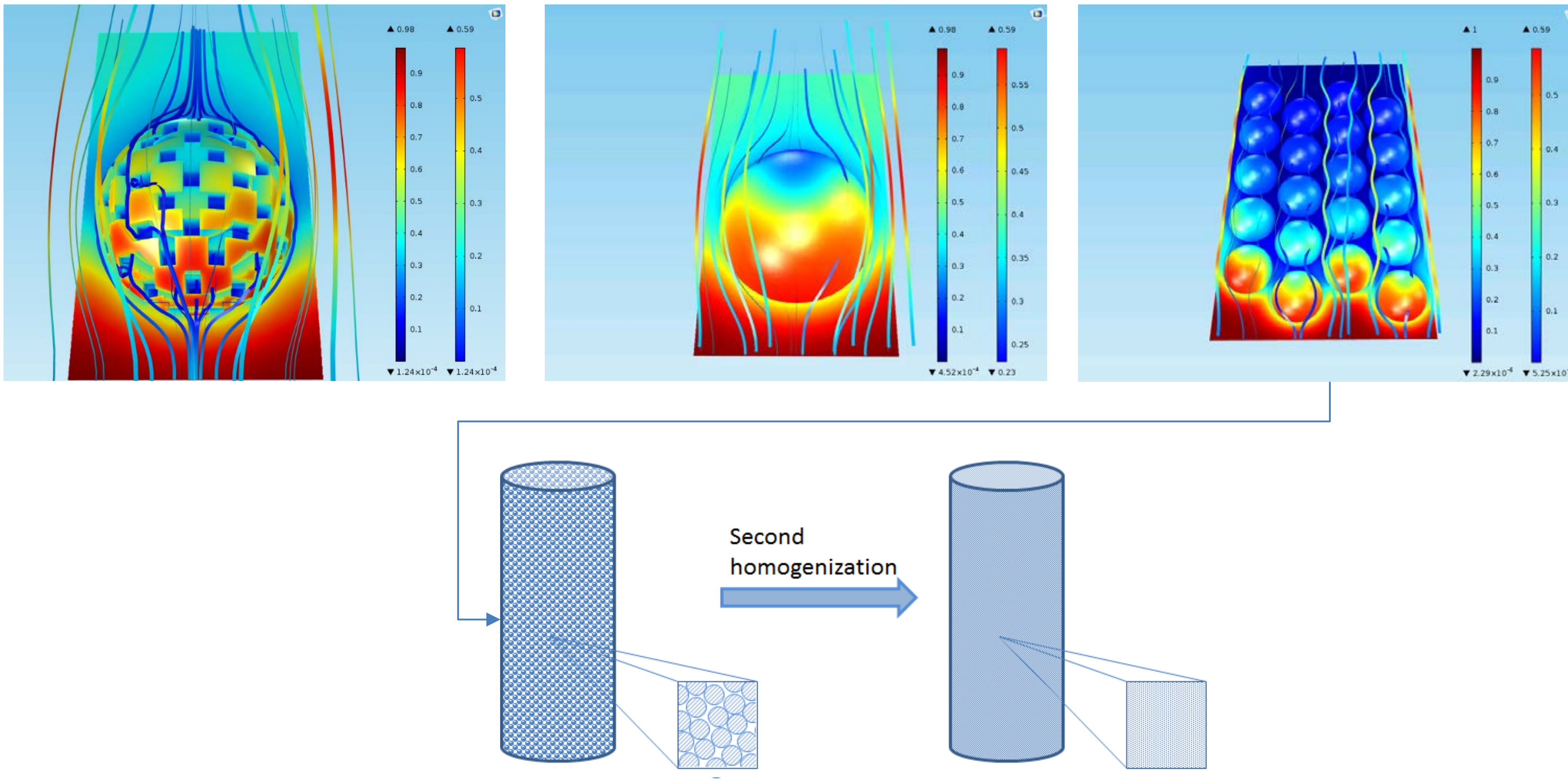
# Model Definition



# Modeling Results

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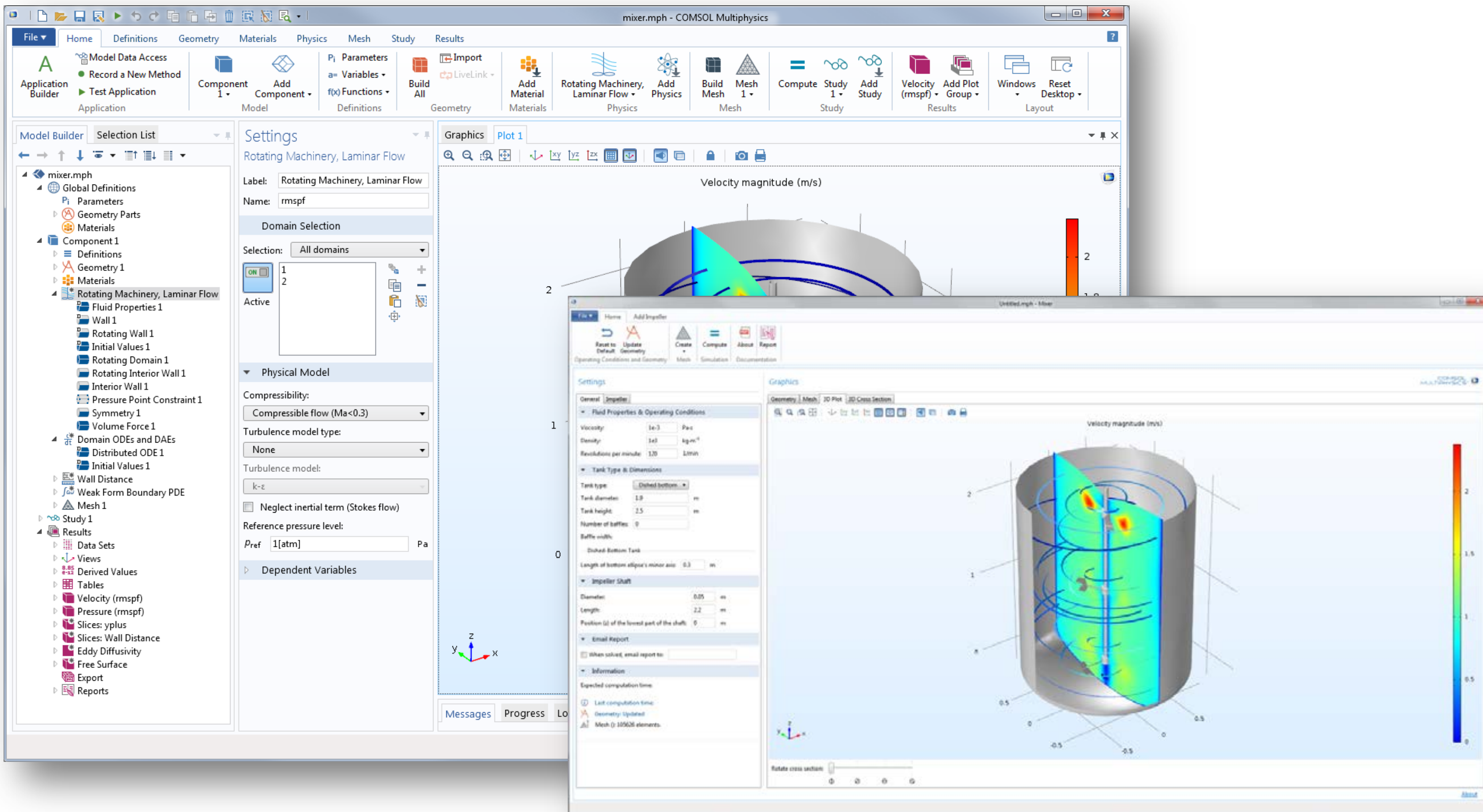
# From Model to App

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# Use of External Physicochemical Data

- CHEMKIN import
  - Standardized text file format for import of
    - Transport properties (viscosity etc)
    - Physical properties (heat capacity, enthalpy, entropy, etc)
    - Reaction kinetics mechanisms (expressions)
  - Set up the reactions automatically in the Reaction Engineering interface
  - NASA Polynomials possible to enter through CHEMKIN™ file

- Thermodynamics interface
  - Port to industrial performance non-ideal mixture property models and data such as
    - Aspen Properties®, aspenONE®, COMThermo® packages, Simulis® Thermodynamics, etc.
  - Temperature- and pressure-dependent properties
  - Concentration-dependent mixing rules (non-ideal mixtures)
  - Multiphase-equilibrium phase diagrams, flash calculations

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# Applications and Examples

# Who can benefit from chemical reaction engineering modeling?

- Not only traditional ”Chemical Industry”:
  - Bulk and Fine Chemicals Production
  - Pulp and Paper
  - Energy and Environmental
  - Food and Household Products
  - Pharmaceuticals and Biotechnology
  - Materials, Polymers, and Petrochemicals
  - Surface Chemistry and Semiconductors
  - Water and Effluent Treatment
  - ...

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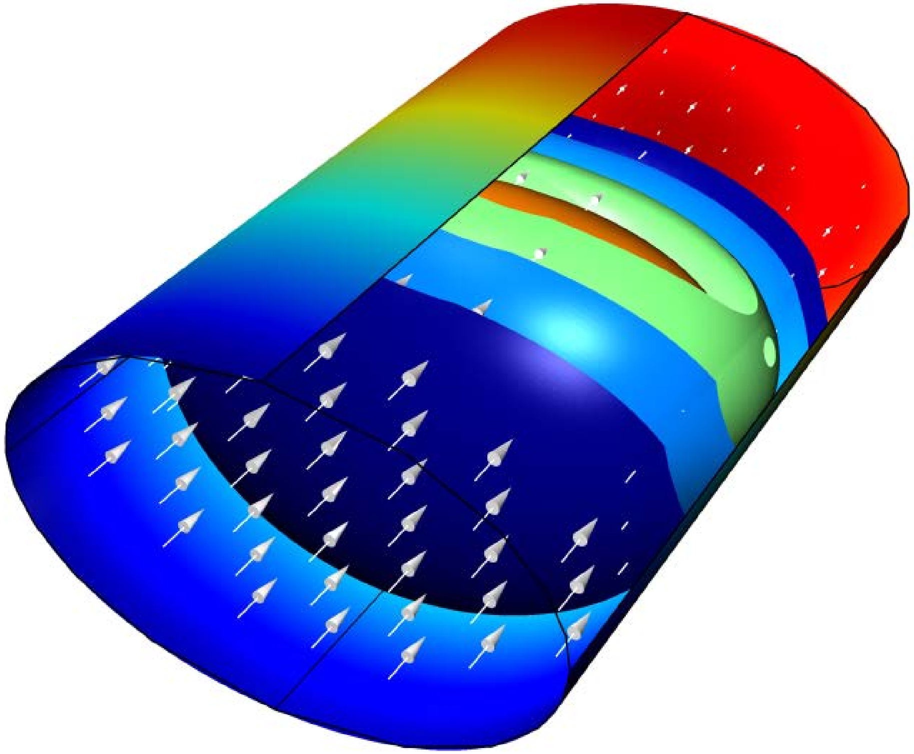
# Energy and Environmental

# Energy and Environmental



Flow field, concentration, and temperature distribution in a diesel particle filter

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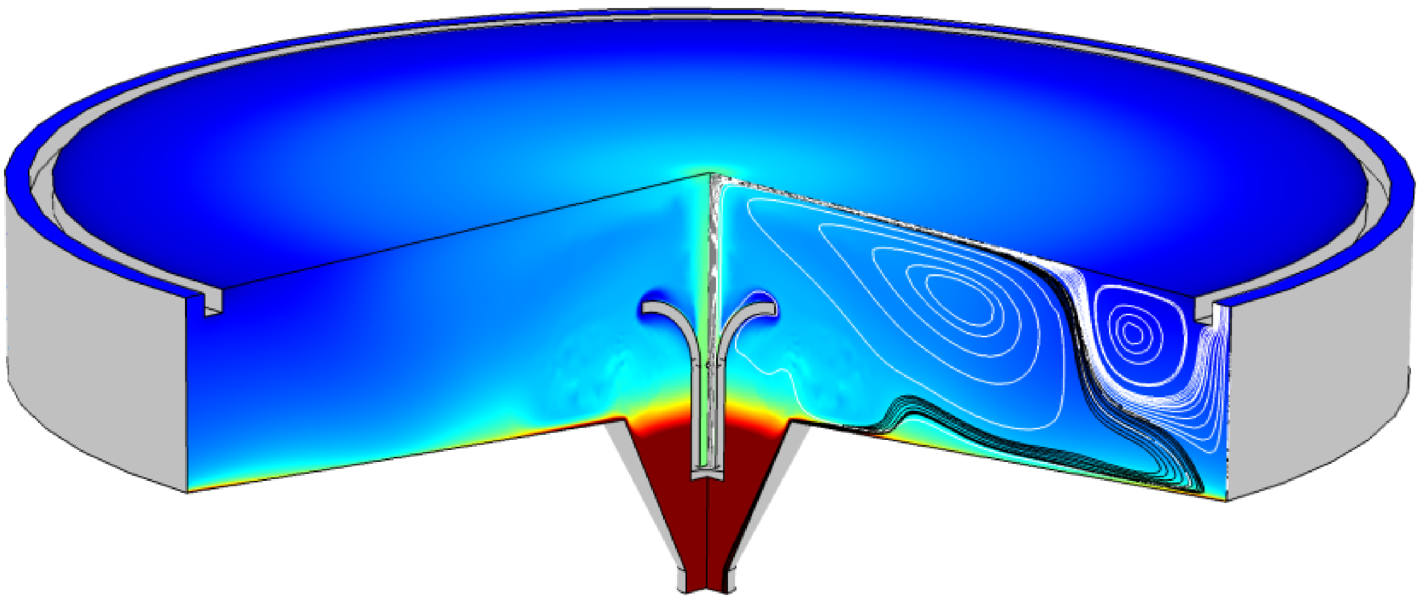
# Water and Effluent Treatment

# Water and Effluent Treatment



* This model also
requires
the CFD Module

Velocity field and volume fraction of the dispersed phase in a secondary sedimentation clarifier*

# Pharmaceuticals and Biotechnology

# Pharmaceuticals and Biotechnology

Temperature distribution and heat flux in a freeze drying process

# Bulk and Fine Chemicals Production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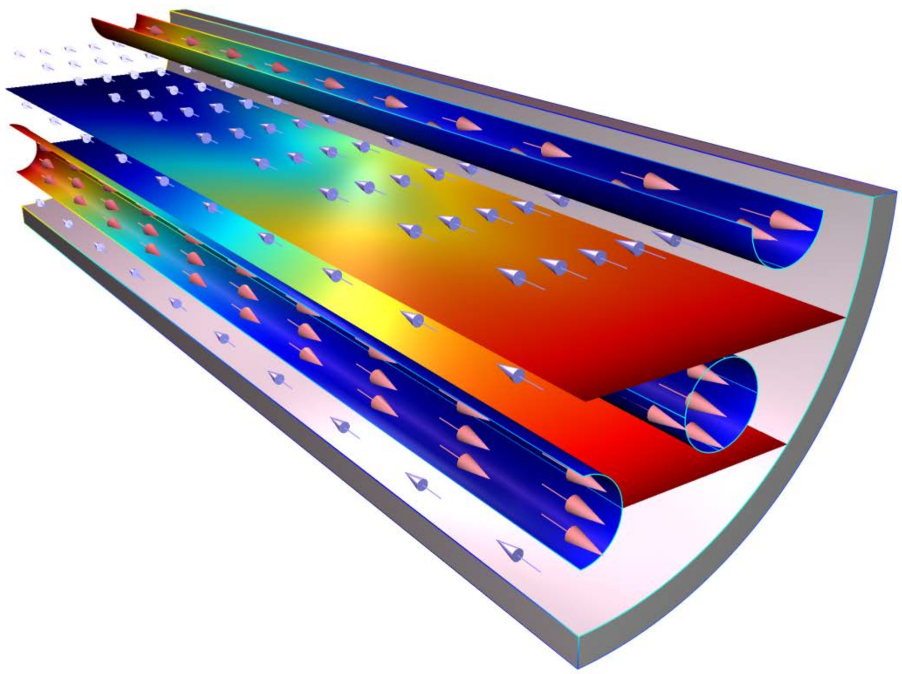
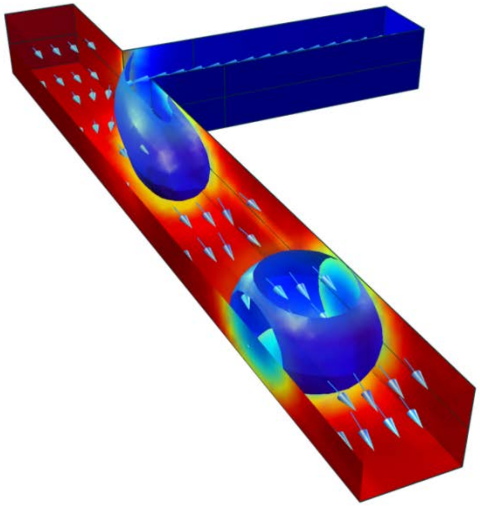
# Bulk and Fine Chemicals Production



Velocity field, concentration, and temperature distributions in a steam reformer

# Food and Household Products

# Food and Household Products



Velocity field and position of the two-phase interface in an emulsifier*

* This model also requires
the Microfluidics Module or the CFD Module

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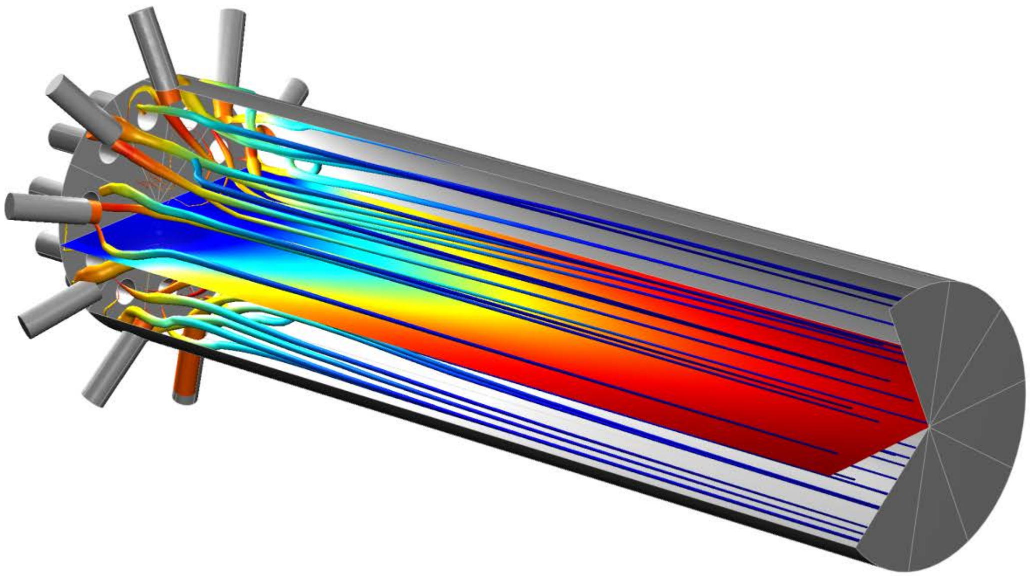
# Petrochemistry and Polymerization

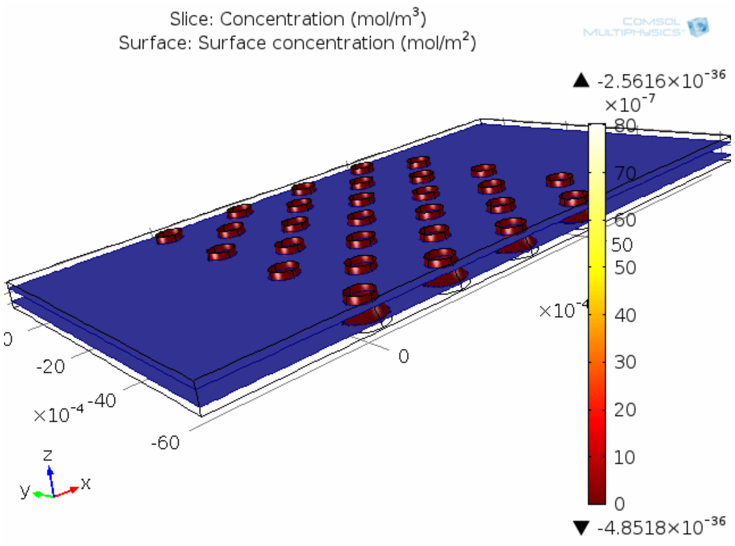
# Petrochemistry and Polymerization

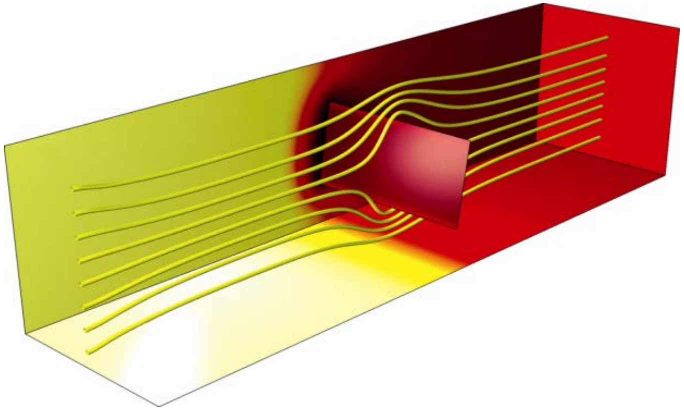


Velocity field and streamlines along with the concentration distribution in a multijet tubular reactor*

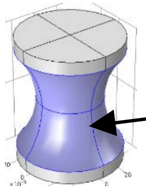
* This model also requires the CFD Module

# Surface Chemistry and Semiconductors



Velocity field streamlines and concentration distribution in a GaAs chemical vapor deposition reactor



Active sites in a biosensor

# Surface Chemistry and Semiconductors

## Bulk reactions

$$Ga(C_2H_5)_3 \xrightarrow{k_1} Ga(C_2H_5)_2 + C_2H_5^{\bullet}$$

$$Ga(C_2H_5)_2 \xrightarrow{k_2} Ga(C_2H_5)H + C_2H_4$$

$$Ga(C_2H_5)H \xrightarrow{k_3} GaH_2 + C_2H_4$$

$$C_2H_5^{\bullet} + H_2 \underset{k_4^r}{\overset{k_4^f}{\rightleftharpoons}} C_2H_6 + H^{\bullet}$$

$$C_2H_5^{\bullet} + H^{\bullet} \xrightarrow{k_5} 2CH_3^{\bullet}$$

$$CH_3^{\bullet} + H_2 \xrightarrow{k_6} CH_4 + H^{\bullet}$$

$$2CH_3^{\bullet} \xrightarrow{k_7} C_2H_6$$

$$C_2H_4 + H_2 \xrightarrow{k_8} C_2H_5^{\bullet}$$

$$2H^{\bullet} + H_2 \xrightarrow{k_9} 2H_2$$

## Surface reactions

$$Ga(C_2H_5)_3 + S_A \xrightarrow{k_{10}} GaC_2H_5^* + 2C_2H_5^{\bullet}$$

$$Ga(C_2H_5)H + S_A \underset{k_{11}^r}{\overset{k_{11}^f}{\rightleftharpoons}} Ga(C_2H_5)H^*$$

$$GaH_2 + S_A \xrightarrow{k_{12}} Ga^* + 2H^{\bullet}$$

$$Ga(C_2H_5)H^* \xrightarrow{k_{13}} Ga^* + C_2H_5^{\bullet} + H^{\bullet}$$

$$AsH_3 + S_G \xrightarrow{k_{14}} As^* + 3H^{\bullet}$$

$$C_2H_5^{\bullet} + S_A \underset{k_{15}^r}{\overset{k_{15}^f}{\rightleftharpoons}} C_2H_{5A}^*$$

$$C_2H_5^{\bullet} + S_G \underset{k_{16}^r}{\overset{k_{16}^f}{\rightleftharpoons}} C_2H_{5G}^*$$

$$C_2H_{5A}^* \xrightarrow{k_{17}} H_A^* + C_2H_4$$

$$C_2H_{5G}^* \xrightarrow{k_{18}} H_G^* + C_2H_4$$

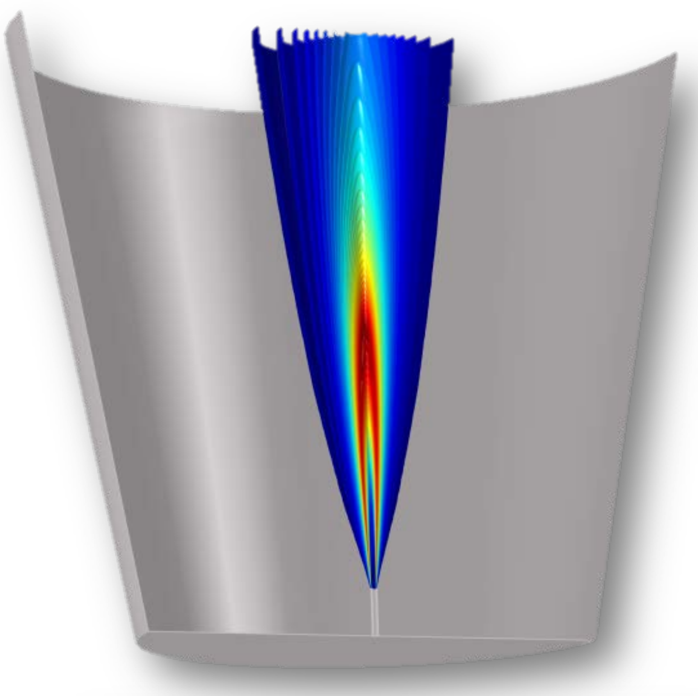
$$H_A^* \xrightarrow{k_{19}} S_A + H^{\bullet}$$

$$H_G^* \xrightarrow{k_{20}} S_G + H^{\bullet}$$

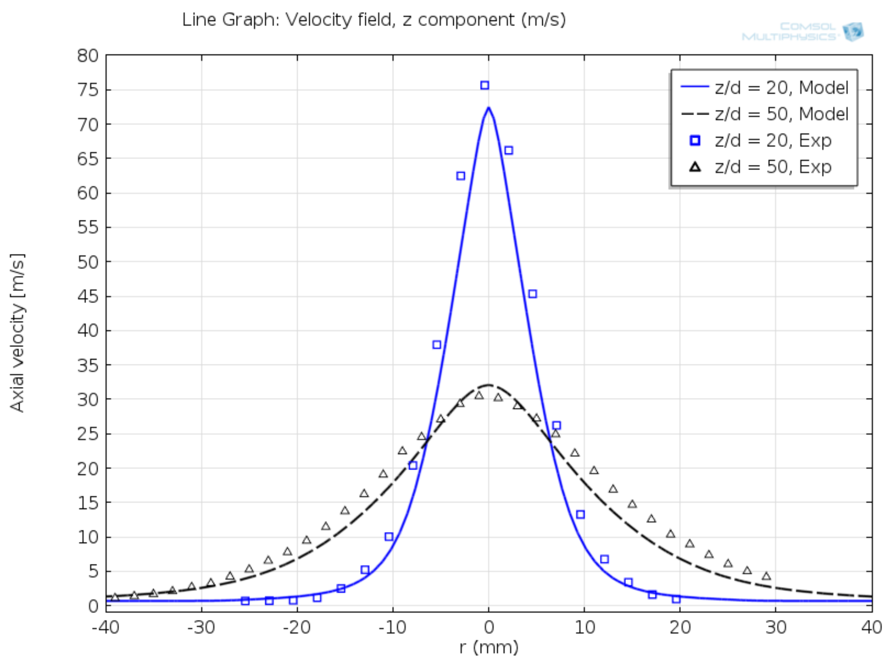
$$GaC_2H_5^* + As^* \xrightarrow{k_{21}} GaAs + C_2H_5^{\bullet} + S_A + S_G$$

$$Ga^* + As^* \xrightarrow{k_{22}} GaAs + S_A + S_G$$

# Combustion Chemistry



COMSOL model of syngas combustion in a turbulent round-jet burner




Good agreement with experimental results

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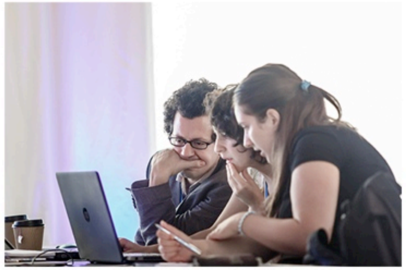

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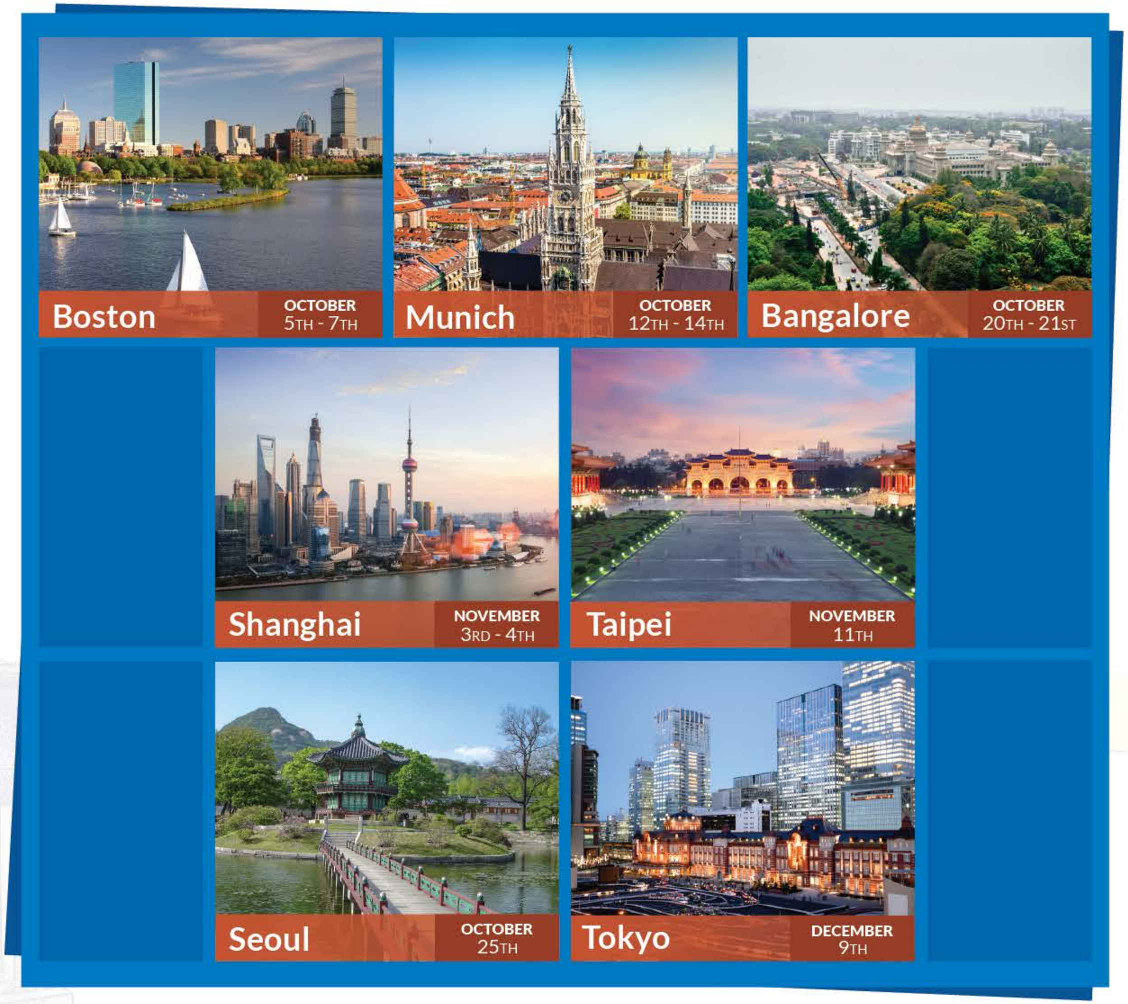


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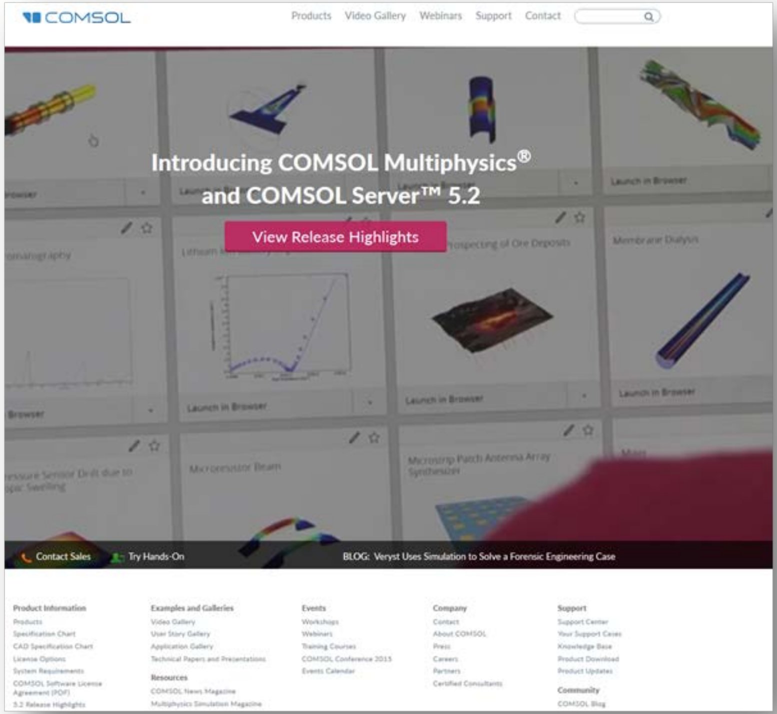


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